ROOT ZONE WATER QUALITY MODEL (RZWQM2): MODEL USE, CALIBRATION, AND VALIDATION

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ABSTRACT. *The Root Zone Water Quality Model (RZWQM2) has been used widely for simulating agricultural management effects on crop production and soil and water quality. Although it is a one-dimensional model, it has many desirable features for the modeling community. This article outlines the principles of calibrating the model component by component with one or more datasets and validating the model with independent datasets. Users should consult the RZWQM2 user manual distributed along with the model and a more detailed protocol on how to calibrate RZWQM2 provided in a book chapter. Two case studies (or examples) are included in this article. One is from an irrigated maize study in Colorado to illustrate the use of field and laboratory measured soil hydraulic properties on simulated soil water and crop production. It also demonstrates the interaction between soil and plant parameters in simulated plant responses to water stresses. The other is from a maize-soybean rotation study in Iowa to show a manual calibration of the model for crop yield, soil water, and N leaching in tile-drained soils. Although the commonly used trial-and-error calibration method works well for experienced users, as shown in the second example, an automated calibration procedure is more objective, as shown in the first example. Furthermore, the incorporation of the Parameter Estimation Software (PEST) into RZWQM2 made the calibration of the model more efficient than a grid (ordered) search of model parameters. In addition, PEST provides sensitivity and uncertainty analyses that should help users in selecting the right parameters to calibrate.*

Keywords. *Hydrological modeling, Modeling, Model validation, Plant growth, RZWQM, Soil water movement.*

The USDA-ARS Root Zone Water Quality Model (RZWQM) was initiated in the middle 1980s and built on knowledge acquired from other system models at that time to improve the simulation of physical, chemical, and biological processes in the root zone (Ahuja et al., 2000a; L. Ma et al., 2000a). These system models included NTRM (Nitrogen Tillage-Residue Management) (Shaffer and Larson, 1987), CREAMS (Chemicals, Runoff, and Erosion from Agricultural Management Systems) (Knisel, 1980), GLEAMS (Groundwater Loading Effects of Agricultural Management Systems) (Leonard et al., 1987), Opus (Smith, 1990), and PRZM (Pesticide Root Zone Model) (Carsel et al., 1985). The first version of RZWQM was released in 1992 and was adopted as the model for the MSEA (Management System Evaluation Areas) project (Watts et al., 1999). A set of articles was published in the *Agronomy Journal* in 1999 (volume 91, issue 2). Although the MSEA project was focused on management effects on soil water quality (pesticide and N) (Wu et al., 1999; Ghidey et al., 1999; Jaynes and Miller, 1999; Martin and Watts, 1999), crop production was also evaluated (Martin and Watts, 1999; Landa et al., 1999).

The second systematic study with RZWQM was focused on pesticides only and was published in *Pest Management Science* in 2004. This special collection of articles started with an overview of the pesticide component in RZWQM by Wauchope et al. (2004), followed by an overview of RZWQM applications for pesticide studies (Malone et al., 2004a). Malone et al. (2004b, 2004c) reported two original studies on pesticide transport in macropores. Pesticide transport to runoff water was documented by Q. Ma et al. (2004a, 2004b). The third major study was published in *Geoderma* (Ahuja and Hatfield, 2007) based on RZWQM applications to long-term experiments at Nashua, Iowa (L. Ma et al. 2007a, 2007b, 2007c; Malone et al., 2007; Saseendran et al., 2007). This set of articles detailed RZWQM applications in simulating management effects on crop production and water quality in tile-drained soils in the U. S. Midwest, including controlled drainage, N application rate and timing, manure application, crop rotation, tillage, and winter cover crop. These *Geoderma* articles complement those published by Dr. Ramesh Kanwar and his students at Iowa State University on RZWQM applications (Singh and Kanwar, 1995a, 1995b; Singh et al., 1996; Kumar et al., 1998a, 1998b, 1999; Bakhsh et al., 1999, 2001,

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2004a, 2004b).

The application of RZWQM in the Central Great Plains was demonstrated in a series of publications on the effect of agricultural management practices (irrigation, fertilization, planting date, and crop rotation) on water use efficiency (WUE) and crop production at Akron, Colorado (L. Ma et al., 2003; Saseendran et al., 2004, 2005a, 2005b, 2007, 2008, 2009, 2010). The calibrated model was also used for soil water content based irrigation scheduling (Saseendran et al., 2008; Fang et al., 2010a) and evapotranspiration (ET) demand based irrigation scheduling (L. Ma et al., 2012). Application of RZWQM for N management and water quality in Portugal and China have been conducted as well (Cameira et al., 2000, 2005, 2007; Fang et al., 2008, 2010a; Hu et al., 2006). A list of publications related to RZWQM is available at www.ars.usda.gov/Main/docs.htm?docid=17740.

The science in RZWQM was documented in a book edited by Ahuja et al. (2000a), and RZWQM applications were reviewed by L. Ma et al. (2000a, 2007d) and Malone et al. (2004a). The science was coded in Fortran and run in DOS mode, but a Windows user interface was developed in C++ in 1998. The model is distributed via the USDA-ARS website at http://arsagsoftware.ars.usda.gov. Source code in Fortran may be obtained from the authors until a permanent location on the website is set up. The user manual was also updated to include interface features and is available with installation of the model and at www.ars.usda.gov/Main/docs.htm?docid=17740. Hints in the manual on how to use the interface to parameterize RZWQM complement the book chapter on protocols for parameterizing RZWQM by L. Ma et al. (2011).

Most of the new components in RZWQM were developed to improve the accuracy of simulations in the crop root zone. As a result, RZWQM contains a detailed soil water and heat transfer module (Ahuja et al., 2000b; Flerchinger et al., 2000), an N balance module (Shaffer et al., 2000a), a generic plant growth module (Hanson, 2000), an extended Shuttleworth-Wallace potential evapotranspiration (PET) module (Farahani and DeCoursey, 2000), a soil equilibrium chemistry module (Shaffer et al., 2000b), a pesticide module (Wauchope et al., 2000, 2004), and a management module (Rojas and Ahuja, 2000). A snow routine was implemented from PRMS (Precipitation Runoff Modeling System) (Leavesley et al., 1983), and the tile drainage component was adapted from DRIANMOD (Skaggs, 1978). Tillage effects on soil bulk density and rainfall effects on soil reconsolidation were taken from the EPIC (Environmental Policy Integrated Climate) model (Williams, 1995). In 2007, an updated version of RZWQM was released as RZWQM2, which contains surface energy balance from the SHAW (Simultaneous Heat and Water) model (Flerchinger and Saxton, 1989; Flerchinger and Pierson, 1991) and the crop growth modules from DSSAT (Decision Support System for Agrotechnology Transfer) (Jones et al., 2003). Recently, the Parameter Estimation Software (PEST) was incorporated into RZWQM2 to facilitate model parameterization (Doherty, 2010).

The objective of this article is to review the key features of RZWQM2, the most commonly calibrated parameters, and steps to calibrate the model for various model applications. Two case studies are provided to illustrate the procedures to calibrate RZWQM2 in two different experimental settings. We also point out the strength and weakness of the model, along with future improvements under consideration.

RZWQM2 Description

RZWQM2 is a point (one-dimensional) model with emphasis on management effects on water quantity, water quality, and crop production. It can simulate a 30 m deep soil profile with at most one crop grown at any given time. The model contains plant growth modules for 22 field crops from the DSSAT crop modules (L. Ma et al., 2011). It runs on a daily time step for crop growth, N balance, and pesticide modules; a subhourly time step is used for soil water, soil heat transfer, and surface energy balance modules. The model allows for ten soil horizons, which may be subdivided up to 300 numerical nodes. The model may accommodate up to 200 events for each management practice (tillage, planting dates, fertilization, manure application, etc.). Thus, the temporal scale of the model depends on the number of events scheduled for each management practice during a simulation run.

Soil Water Balance Module

The modified forms of the Brook-Corey equations (see Appendix A) are used for describing soil water retention curves in RZWQM2 (Brooks and Corey, 1964). The Green-Ampt equation is used for infiltration during rainfall or irrigation (snowmelt is treated as irrigation), and the Richards equation is used for redistribution between rainfall or irrigation events (Ahuja et al., 2000a). Plant water uptake is treated as a sink term in the Richards equation and estimated by the Nimah-Hanks equation (Nimah and Hanks, 1973) or an empirical function in DSSAT crop modules. Estimated plant water uptake is then limited by potential transpiration calculated from the extended Shuttleworth-Wallace potential evapotranspiration (PET) module (Shuttleworth and Wallace, 1985; Farahani and Ahuja, 1996). Tile drainage flow is also treated as a sink term and calculated from Hooghoudt's steady-state equation as implemented in the DRIANMOD model by Skaggs (1978). The mass-conservative, mixed-form, iterative finite difference method of Celia et al. (1987, 1990) is used to solve the Richards equation (Ahuja et al., 2000b). The upper boundary for the Richards equation may be flux based according to potential evaporation rate from the extended Shuttleworth-Wallace PET module or constant head when the soil water suction is at wilting point (1500 kPa suction) or greater. The lower boundary may be unit gradient for unsaturated flow or constant flux when a water table exists.

Macropore flow capacity (maximum flow rate) is simulated in RZWQM2 using Poiseuille's law based on gravity flow. Water absorption by the soil matrix around the macropores is computed by radial or lateral Green-Ampt equation for cylindrical pores or cracks, respectively. Water enters the macropores only at the soil surface when the rainfall or irrigation rate exceeds the simulated infiltration rate. If overland flow is still available, water exits the field as runoff. Surface water detention is not simulated at this time. Chemicals entering macropores are estimated from their concentration in the overland flow, which is calculated from the non-uniform extraction model of Ahuja (1986).

SOIL NUTRIENT MODULE

Nitrogen is the only nutrient simulated in RZWQM2. The model divides organic N into five pools, i.e., fast and slow residue pools and fast, intermediate, and slow soil humus pools. The humus pools are commonly called soil organic matter. Three microbial pools (aerobic heterotrophs, autotrophs, and anaerobic heterotrophs) mediate the transfer and decomposition of the five organic pools (Shaffer et al., 2000a). Each pool has a fixed C:N ratio. Organic carbon is the backbone of soil C:N transformation. Mineralization or immobilization of N is calculated from the amount of C mineralized and the C:N ratio of the pools. Aerobic decay of organic pools to ammonium (NH_4) by heterotrophs is assumed to be a first-order reaction with its constant as a function of soil temperature, soil moisture, soil pH, and microbial population. Urea may also be hydrolyzed to ammonium. The resulting ammonium is then nitrified to nitrate (NO_3) by autotrophs. Under anaerobic conditions, nitrate can be denitrified to N_2O and N_2 by anaerobic heterotrophs. The aerobic or anaerobic condition is determined by percent water-filled pore space (PWFPS). All these processes are simulated as first-order reactions.

Under anaerobic conditions when denitrification occurs, a portion of the organic carbon is decomposed to supply energy for the growth of anaerobic heterotrophs. This is called anaerobic decay of soil organic matter and is proportional to the rate of denitrification. The growth of heterotrophs is proportional to the decay rate of organic matter, and the growth of autotrophs is proportional to the nitrification rate. Microbial death is proportional to its respective population. However, users have the option to turn off the microbial growth and use constant microbial populations provided in the model. Ammonia volatilization is modeled based on the partial pressure gradient of NH_3 between the soil and air (Shaffer et al., 2000a). The model also considers a delay in nitrification due to microbial recovery around the nozzles where anhydrous ammonia is applied. Nitrification can be further delayed when an inhibitor is used.

EQUILIBRIUM SOIL CHEMISTRY MODULE

The equilibrium soil chemistry module in RZWQM2 has not been fully tested thus far. It is designed to simulate long-term effects of agricultural management on soil pH and salinity. It includes cations such as H^+, Ca^{2+}, Mg^{2+}, Na^+, NH_4^+, and Al^{3+} and anions such as SO_4^{2-}, CO_3^{2-}, OH^-, NO_3^-, and Cl^-. The chemical reactions are assumed to be at equilibrium in the soil solution, given that these reactions are concurrently fast processes. Various ion pairs are also considered, such as $NaSO_4^-$, HCO_3^-, $AlSO_4^+$, and $AlOH^{2+}$. Solubility equations are used for dissolution and precipitation of partially soluble salts, such as gypsum, calcium carbonate, and gibbsite. Ion exchange equations are included for adsorption-desorption of cations in solution and on the soil surface. The system of equations is solved with the Newton-Raphson algorithm (Shaffer et al., 2000b). Because this module is the least evaluated module in RZWQM2, its use will not be illustrated in this article.

POTENTIAL EVAPOTRANSPIRATION, SURFACE ENERGY BALANCE, AND HEAT TRANSFER MODULE

RZWQM2 uses the Penman type (Shuttleworth-Wallace) surface energy balance to calculate potential evaporation for the upper boundary condition in solving the Richards equation and potential transpiration as the upper boundary for plant water uptake. Heat transfer during rainfall or irrigation events results from water movement in the soil profile. During redistribution, the convective-dispersive heat equation is solved for heat transfer. The upper boundary condition is assumed to be air temperature on the soil surface. A Neumann type-2 lower boundary condition is assumed at the bottom of the soil profile. With SHAW incorporated into RZWQM2, users have the option to use the SHAW surface energy balance module that simulates all energy components (total radiation, sensible heat, latent heat, and soil ground heat flux). This new module will provide a more realistic soil surface temperature, especially for residue and canopy covered surfaces, and has the ability to simulate canopy temperature and energy fluxes within a crop canopy (Flerchinger and Saxton, 1989; Flerchinger and Pierson, 1991).

PESTICIDE PROCESSES MODULE

The pesticide module in RZWQM2 is complex yet practical. It provides users with the ability to include pesticide application efficiency, pesticide interception by foliage and crop residue, and slow-release form of the pesticide (Wauchope et al., 2000, 2004). Pesticide retained by foliar and crop residue may be washed off onto the soil surface as a function of rainfall and degraded according to a first-order reaction. Pesticide may be adsorbed and degraded in the soil. Adsorption of pesticide may be equilibrium or kinetic in nature according to the user's selection. A fraction of the absorbed pesticide can become irreversible with time. Soil degradation coefficients (in terms of half-lives) of pesticides may be a function of soil depth, soil pH, soil temperature, and soil water content. Another unique feature of the model is its ability to simulate daughter and granddaughter products due to pesticide degradation. So far, the model can simulate up to three species of pesticides with any combinations of parent, daughter, and granddaughter, e.g., 3 parents, 1 parent + 2 daughters, or 1 parent + 1 daughter + 1 granddaughter.

PLANT GROWTH MODULES

RZWQM2 originally had a generic plant growth module that could be parameterized for any annual crop (Hanson, 2000). It is currently parameterized mainly for maize, soybean, and winter wheat, although a study on cotton was published in the literature (Abrahamson et al., 2005). This module simulates above and below ground biomass, yield, and phenology. It simulates water and N uptake from soils in water quality experiments. Since this module takes considerable experience and knowledge to parameterize for a new crop, a growth curve approach was added to the model to simulate only plant water and N uptake without considering plant growth. Recently, the DSSAT crop growth modules (version 4.0) were linked to RZWQM2 so that the model can be used for better simulation of crop production in addition to soil water and water quality (L. Ma et al., 2005, 2006), which extended simulated crops to 22 along with an extensive database for crop parameters. Each crop requires only a few parameters to calibrate. Therefore, it is easier to use than the original generic plant growth model in RZWQM2. Details of the DSSAT model can be found in Jones et al. (2003).

Plants can take up both NH_4 and NO_3 proportionally based on their concentrations in soils. Plant N demand is calculated from daily C assimilation and N concentration in the new growth, and actual N uptake is constrained by soil N supply. For legumes, N fixation kicks in when soil N supply cannot meet plant N demand. In the generic plant growth module, the difference between plant N demand and soil N supply is met fully by N fixation without simulating the process of N fixation. However, there is an N fixation module in the DSSAT crop models to calculate daily N fixation by simulating nodule growth.

Management Practices Module

The ability to simulate a wide range of agricultural management practices was another goal in developing RZWQM2. Tillage effects on soil properties and plant growth is one of the main practices simulated (Rojas and Ahuja, 2000). Another important management practice is manure and fertilizer application, including amount and timing. The third main practice is water management, such as timing and amount of irrigation. RZWQM2 also provides rule-based water and N management. Fertigation and chemigation are also included in the model.

RZWQM2 Calibration and Validation

RZWQM2 is a system model that requires extensive input data, such as weather (air temperature, solar radiation, relative humidity, wind speed, and rainfall), soil information (hydraulic, physical, chemical, and heat properties), and management practices (irrigation, fertilization, pesticide application, plant management, and tillage). First, a model user should collect all the above information and conduct a quality check of the data (Malone et al., 2011). RZWQM2 can accept both hourly and daily weather inputs, so users should decide which resolution of weather data they want to use. In general, hourly weather data are preferred over aggregated daily data.

Second, measured data should be identified for model calibration and model validation purposes. There are seldom any experiments that measure all the components or processes of an agricultural system due to limitation of time and resources. A model user has to make the best use of existing data to calibrate a model to a certain level of satisfaction and use the rest for model validation. Quality control of the experimental data should also be performed.

Third, model parameters need to be identified for calibration. It is recommended to calibrate the parameters that either cannot be measured or measured with less confidence (due to instrumentation failure or spatial/temporal variability). Although it is a commonly accepted practice to use the data under the least stressed conditions for model calibration in a cropping system, users should also identify a dataset with balanced measurements of all system components (i.e., both soil and plant), high temporal and spatial resolution, and high accuracy. For model evaluation or validation, at least one dataset under stressed condition should be used to show model sensitivity to the treatments of interest. It is not desirable to use one year of data for calibration and another year of data for model validation, with a single treatment involved, because the two years may have similar weather conditions.

It is desirable to calibrate a system component with minimum interference (or interactions) from other components. For example, when there is a fallow period in a crop system, soil properties should be calibrated in the fallow phase and the plant parameters in the crop phase. Since there is a strong interaction among system components, an iterative calibration procedure among system components should be followed (L. Ma et al., 2011). This iterative procedure is also required due to the large degrees of freedom in model calibration. In addition, since there are multiple sets of model parameters that may produce similar results, including measurements from multiple years and multiple treatments should reduce the degree of freedom in model calibration (L. Ma et al., 2012). In RZWQM2, it is recommended to start calibration with soil water, followed by soil nutrient or pesticide and plant growth, and then recalibrate in the same order. Two or three iterations are usually required to come up with an acceptable set of parameters.

Table 1 lists the minimum measurements required for calibrating each system component, and table 2 lists the minimum inputs needed to run the calibrated RZWQM2. It should be noted that these minimum measurements should have a reasonable resolution in space and time as well. When only minimum data are available, it is important to check all model outputs to make sure their values are reasonable for the given soil and climate conditions, even though there are no experimental measurements (table 3). A more complete dataset to calibrate RZWQM2 is listed in table 4.

Table 1. Minimum measurements required to adequately calibrate a system component.

System Component	Prerequisite System Component	Measurement
Soil water balance	-	Soil water content
Soil nitrogen (N) balance	Soil water	Soil N concentration, plant N uptake, soil organic matter content
Pesticide component	Soil water	Soil pesticide concentration
Plant growth	Soil water, soil N	Yield, aboveground biomass, leaf area index (LAI), phenology
Surface energy balance	Plant growth	Soil temperature, soil water content, LAI, plant height, plant biomass

Table 2. Minimum data required to run RZWQM2.

Data Type	Minimum Data Required
Rainfall	Amount and intensity.
Daily or hourly weather	Daily meteorology data (minimum and maximum air temperature, wind run, solar radiation, and relative humidity).
Site description	Latitude, elevation, longitude, and slope.
Soil properties	Soil horizon delineation, soil texture, and bulk density. Optional soil hydraulic properties: soil water content at 33 and 1500 kPa suction, and saturated hydraulic conductivity (K_{sat}).
Pesticide properties	General pesticide data such as common name, half-life, adsorption constant (K_d), and dissipation pathways.
Plant	Specifying a crop cultivar from supplied database.
Management practices	Estimate of dry mass and age of residue on the surface, tillage, irrigation, planting/harvest, fertilization, etc.
Initial soil conditions	Initial soil water content/water table; initial soil temperatures; initial soil pH and CEC (cation exchange capacity) values; and initial nutrient model inputs (soil residue, humus, microbial populations, mineral NO_3-N, and NH_4-N).

Table 3. Processes and variables that should be checked in system model outputs (from L. Ma et al., 2011).

Annual or total soil N balance	Initial soil N (organic and inorganic)
	Ending soil N (organic and inorganic)
	N loss to runoff/erosion
	N loss to leaching
	N loss to denitrification
	N inputs (crop residue, fertilizer, and manure)
	Annual N mineralization
Annual or total plant N balance	Total N uptake
	N in root
	N in grain
	N in biomass
	N returned to soil at harvest
	N fixation
Annual or total water balance	Initial soil water
	Ending soil water
	Runoff
	Seepage
	Evapotranspiration
	Subsurface drainage (tile flow)
	Water inputs (rain, irrigation, water table)
Annual or total soil chemical balance	Initial amount
	Ending amount
	Loss to runoff
	Loss to leaching
	Loss to air
	Loss to tile flow
	Chemical input

RZWQM2 has built-in tools to help model parameterization. The pedon database provides first estimates of soil properties based on soil classification. When soil texture is available, refined soil hydraulic properties can be obtained from Rawls et al (1982). These parameters can be improved further if soil water contents at 33 kPa suction ($\theta_{1/3}$) and/or 1500 kPa suction (θ_{15}) are known. When saturated soil hydraulic conductivity (K_{sat}) is unknown, it can be estimated from soil texture based on Rawls et al. (1982) or effective porosity (Ahuja et al., 1989; Ahuja et al., 2010).

A weather generator, CLIGEN, is provided to create weather files when measured weather data are not available. CLIGEN contains all the major weather stations in the U.S. (Nicks et al., 1995). A pesticide database is included in RZWQM2 to provide initial values for pesticide chemistry (Wauchope et al., 1992). The model has a wizard to initialize soil organic pools. Default parameters related to tillage, manure management, and surface energy balance are also provided in the model.

In general, RZWQM2 is calibrated manually by trial-and-error. Therefore, two different users may come up with somewhat different sets of parameters for the same dataset (L. Ma et al., 2008). A recent linkage of PEST (Doherty, 2010) to RZWQM2 enhances the parameterization capability of the model considerably (Nolan et al., 2011; Fang et al., 2010b; Malone et al., 2010). Users can select which parameter or which group of parameters to optimize by giving each parameter a range to sample from. Users can also emphasize one or more model outputs (e.g., yield, biomass, soil moisture content, etc.). However, users need to carefully select the weighting factor for each model output in constructing an overall objective function to optimize. A poor selection of the weights may cause the objective function to oscillate without improving simulation results.

Sensitivity analysis can aid model parameterization by identifying the most sensitive parameters, especially when less is known about the parameters. A procedure similar to manual calibration can be used for sensitivity analysis. However, sensitivity of a parameter depends on soil, weather, and management conditions as well as output variables of interest (L. Ma et al., 2000b). Users should conduct a sensitivity analysis for the parameters of interest and focus calibration on the most sensitive ones. PEST (Doherty, 2010) features sensitivity and uncertainty analyses along with autocalibration. During calibration, PEST computes derivatives of model predictions with respect to the parameters to determine the magnitude and direction of parameter adjustment. This matrix is called the Jacobian, or sensitivity, matrix. When optimization is complete, composite sensitivities for each parameter are written to a sensitivity output file, and these indicate the relative importance of the parameters.

PEST includes a suite of utilities to perform linear pre-

Table 4. A more complete experimental dataset for RZWQM2 calibration (both inputs and outputs).

Data Group	Data Element
Soil property	Bulk density; soil water retention curve; saturated soil hydraulic conductivity; soil horizons.
Water balance	Soil water content; runoff water; water seepage or drainage; evapotranspiration.
N balance	Soil N concentration; N in runoff, seepage, and drainage; plant N uptake; annual soil organic N mineralization.
Pesticide	Soil pesticide concentration; pesticide in runoff, seepage, and drainage; plant uptake of pesticide; pesticide on foliar and crop residue.
Energy balance	Soil and canopy temperature; net radiation, latent heat, sensible heat, and soil heat flux.
Plant	Yield; biomass; LAI; plant height; phenology; leaf number, tiller number; yield components; rooting depth.

Table 5. Choice of parameters and variables to be considered for calibration for various processes or outcomes (from L. Ma et al., 2011).[a]

Processes or Outcomes	Related Parameters or Variables
Soil water dynamics	Brooks-Corey parameters, especially $\theta_{1/3}$ and θ_{15}, pore size distribution index (λ), bubbling pressure (h_b), N_2, and K_{sat}, bulk density or porosity, water inputs to the soil and losses from the soil including plant water uptake.
Runoff	K_{sat} at surface layer, rainfall intensity, presence of macropore flow, and surface crusting.
Tile flow	K_{sat} and lateral K_{sat}, tile spacing and depth, lateral flow below tile controlled by a lateral hydraulic gradient, drainable porosity (porosity – $\theta_{1/3}$) and water table leakage rate.
Water table fluctuation	K_{sat} at lower soil layers, tile flow amount, lateral flow below the tile lines, and leakage rate.
Evapotranspiration	Albedos, residue cover, LAI simulation, stomatal resistance, soil surface resistance to vapor flux, and rooting depth.
Water uptake	Potential evapotranspiration (PET), rooting depth, soil water content, $\theta_{1/3}$ and θ_{15}, K_{sat} by layers, and soil root growth factor (SRGF).
N uptake	N supply from soil, N demand from daily plant growth as defined by N concentrations in each tissue, and passive uptake through transpiration and active uptake parameters.
Annual N mineralization	Soil carbon (C) pool partitioning, interpool transfer coefficients, crop residue returned to the soil, decomposition rates of each pool if needed, and mechanical and biological mixing of crop residues into soil.
Soil inorganic N (NO_3 and NH_4) dynamics	Plant N uptake, N leaching, denitrification, volatilization, nitrification, and hydrolysis rate constants, and N applications and methods.
Plant development	Thermal time or minimum days between growth stages.
Plant biomass accumulation	Daily photosynthesis rate, length of vegetative growth, plant water/N stresses, and rooting depth.
Plant yield formation	Yield formation parameters, such as maximum kernel number, kernel weight, daily partitioning of biomass to yield (generic growth model), grain filling duration and rate, length of reproductive growth, and plant water/N stresses.
Rooting distribution	Maximum rooting depth, relative SRGF in each layer, and partitioning of photosynthate to root (generic growth model).
Pesticide processes	Adsorption constant, kinetic adsorption, macropore flow, volatilization, runoff loss, leaching loss, and plant uptake.

[a] K_{sat} is saturated soil hydraulic conductivity, $\theta_{1/3}$ and θ_{15} are soil water content at 33 and 1500 kPa suction, respectively, and N_2 is the exponent for the soil hydraulic conductivity and soil water suction head curve.

dictive uncertainty analysis, which is more computationally efficient than nonlinear approaches (Doherty et al., 2010). For example, the PREDUNC utilities estimate predictive uncertainty and parameter contributions to predictive uncertainty. The utilities are easy to use because they require only a PEST control file, a Jacobian matrix file, and (optionally) a parameter uncertainty file. The utilities use a Bayesian approach that updates an *a priori* estimate of parameter uncertainty by information gained through calibration (Fienen et al., 2010). The posterior uncertainty component is based in part on the epistemic uncertainty of the observations, which includes measurement error, model error, and other nonrandom sources of error.

Since a model cannot be verified, the term validation is used in the context of using a different dataset than that used for model calibration. In the literature, selecting which dataset for calibration and which dataset for validation varies from user to user. Some users use one treatment for calibration and the rest for validation (Hu et al., 2006), and some use all treatments in one year for calibration and the other years for validation (L. Ma et al., 2003). Based on L. Ma et al. (2012), model calibration should include multiple years and multiple treatments so that the calibrated model parameters are more robust. In this case, model calibration and validation are embedded into the iteration process of model parameterization.

Calibration Parameters

L. Ma et al. (2011) recommended the parameters to calibrate for each system component (table 5). Ideally, each model parameter should be obtained independently. When there is uncertainty in input parameters, a model should be run under the distribution of each parameter rather than a single value. In this case, the model output is a distribution as well, which can be compared directly with field-measured values and associated errors. Table 6 lists some of the model parameters calibrated in various studies in the literature.

Parameters for Soil Water Balance

Soil water content is one of the most commonly measured data available in field research. The soil water retention curve (Brooks-Corey equation in RZWQM2) and saturated soil hydraulic conductivity (K_{sat}) have the most effect on soil water distribution in the soil. The model provides average values for these parameters based on soil texture as default values if measurements are not available. The easiest way to calibrate the Brooks-Corey parameters is to adjust soil water contents at 33 kPa ($\theta_{1/3}$) and 1500 kPa (θ_{15}) suction. Measured K_{sat} usually has high standard error, so it may be calibrated to improve soil water simulation. The K_{sat} can be estimated from saturated and 33 kPa water contents (θ_s – $\theta_{1/3}$) (Ahuja et al., 1989, 2010). Soil bulk density determines saturated soil water content (θ_s), so it should be calibrated if needed. Rooting depth should be reasonable for water extraction from each soil layer. Other processes that affect soil water content are soil evaporation, crop transpiration, surface runoff, snowmelt, deep drainage, and tile flow (L. Ma et al., 2011).

Subsurface drainage (tile flow) is affected by lateral hydraulic conductivity (LK_{sat}), water table, drain spacing, and depth of the drains. It is important to maintain a water table within the soil profile throughout the simulation. Once the water table recedes below the bottom of the soil profile, it cannot be brought back to the system. Therefore, users should extend their soil profile to encompass the soil water table at all times. An impermeable soil layer at the lowest soil depth is important for building a water table. RZWQM2 also has a pseudo-lateral flow below the drainage tiles, which is controlled by a user-defined lateral hydraulic gradient. Increasing this lateral flow will lower the water table and subsequently tile flow.

Runoff in RZWQM2 is produced only when the rate of rain or irrigation exceeds simulated soil infiltration rate and macropore flow capacity. Therefore, calibration of surface K_{sat} (even adding a surface soil crust) may be needed for runoff water calibration. Another important factor for run-

Table 6. Examples of calibration in RZWQM applications (adapted from L. Ma et al., 2011).

Parameters Calibrated	Measurements to Match	Authors
Saturated soil water content and hydraulic conductivity, macroporosity, fraction of dead macropores	Water redistribution and infiltration	Cameira et al. (2000, 2005) and Kumar et al. (1998a)
Stomatal and soil resistance, maximum rooting depth	Evapotranspiration	Cameira et al. (2005) and L. Ma et al. (2003)
Soil carbon pool size, nitrification and urea hydrolysis rate coefficients	Total soil C, soil nitrate distribution and plant N uptake	Cameira et al. (2007)
Interpool transfer coefficients among soil carbon pools	N loss in tile flow, soil N distribution	Malone et al. (2010) and L. Ma et al. (1998)
Lateral hydraulic gradients and lateral hydraulic conductivity, Brooks-Corey soil water retention parameters	Tile flow	Malone et al. (2010), L. Ma et al. (2007a), Nolan et al. (2010), and Qi et al. (2011)
K_{sat}, Brooks-Corey soil water retention parameters, bulk density	Percolate from soil block, soil water distribution	Malone et al. (2003), Sophocleous et al. (2009), Nolan et al. (2010), and L. Ma et al. (2012)
K_{sat} for crusted soil surface	Surface runoff	Q. Ma et al. (1995, 2004a)
Field capacity and/or wilting point	Soil water content	L. Ma et al. (2003), Hu et al. (2006), and Fang et al. (2010a)
Soil hydraulic parameters, interpool transfer coefficient between the intermediate and the slow organic pools	Soil water content, soil water tension, bromide and nitrate in lysimeters, soil organic matter content	Nolan et al. (2010)
Porosity and field capacity	Subsurface drainage	Kumar et al. (1998a) and Bakhsh et al. (2004a)
Pesticide adsorption constant and pesticide half-life	Pesticide loss in tile drainage	Bakhsh et al. (2004a)
Macroporosity	Till and no-till effects on pesticide leaching	Malone et al. (2004b)
Soil root growth factor (SRGF)	Plant growth, soil water content distribution	Malone et al. (2010), Fang et al. (2010a), and Nolan et al. (2010)
Lateral sorptivity factor to macropore walls	Pesticide leaching into tile flow	Kumar et al. (1998a) and Malone et al. (2001)
Non-uniform mixing factor for chemical extraction	Chemical in runoff	Ghidey et al. (1999) and Malone et al. (2001)
Soil horizon depth	Soil water content and N	Martin and Watts (1999)
Albedo	Soil water content	Nokes et al. (1996)
Initial soil water content if not measured	Pesticide soil distribution, tile flow	Azevedo et al. (1997) and Singh et al. (1996)
Washoff factor and macropore radius	Pesticide leaching	Malone et al. (2001)

off is the rainfall intensity. Subhourly rainfall intensity may be required for a reliable runoff calibration.

Parameters for Soil Energy Balance and Heat Transfer

Soil temperature is a result of surface energy balance and water movement. In RZWQM2, plant, residue, and soil albedo can be calibrated to improve surface energy balance simulations. The model calculates heat capacity and heat conductivity based on soil texture and soil water content. An option to use the detailed energy balance module of SHAW should be selected when high accuracy of soil surface temperature simulation is desirable and simulation of canopy temperature and soil freezing is important. Correct simulation of canopy cover is a prerequisite for good energy balance simulation. Details on calibrating the SHAW model can be found in Flerchinger et al. (2012).

Parameters for Soil Nitrogen Balance

Partitioning of the soil organic matter into pools is important for mineralization of organic N. Initializing these pools (organic and microbial pools) should be done based on recommendations in the user's manual by running the model for 10 to 12 years with current or previous management practices (L. Ma et al., 1998). When urea is applied, the rate of its hydrolysis may be calibrated for correct transformation of urea to NH_4. When anhydrous ammonia is applied, the rate of ammonia volatilization should be calibrated. Soil NH_4 and NO_3 distributions are affected by inputs from N mineralization and fertilization, N leaching, plant N uptake, and immobilization to microbial biomass. Plant N uptake, N fixation, and root distribution in the soil profile are important in calibrating soil N balance.

Parameters for Pesticide Movement

Application efficiency of pesticide spray varies greatly from experiment to experiment depending on weather conditions and soil surface cover. Users should verify the actual amount of pesticide reaching the crop canopy and soil surface by taking samples as soon as spraying is finished. The equilibrium adsorption constant of pesticide in soil is one important parameter to calibrate. When kinetic adsorption is necessary for a pesticide, users should also calibrate the kinetic reaction rate as well. Degradation constants (input as half-lives) of pesticide on the foliar, crop residue, and soil should be calibrated as well. A fraction of the adsorbed pesticide may become irreversible (treated as dissipation in RZWQM2 and computed by a user-defined half-life). When soil macropore exists, pesticide transport via macropore is affected by macropore size and the thickness of the macropore walls.

Parameters for Plant Growth

After soil water and soil nutrient are reasonably calibrated, users can then look at plant growth parameters. The first step is to calibrate plant phenology for reasonable simulation of plant germination, anthesis, and physical maturity dates. These dates are important in simulated plant development and plant response to water, nitrogen, and heat stresses. For the DSSAT crop growth modules, there are separate parameters for calibrating phenology and production. All the parameters related to the species of the crop are in the species file, which may be changed by experienced users. The second file is the ecotype file, which contains parameters common to a group of crops in that species and should only be changed by experienced users. The last file is the cultivar file, which applies to a particular crop variety; users should focus on these parameters to calibrate plant growth. It is important to view the simulated water and N stresses to make sure that the simulated stresses are in agreement with field observations. When an abnormal stress is simulated, users should check water and N balances to eliminate any mistakes in model inputs or related parameters. For the generic crop growth module, some common parameters are managed by the user interface, and others are in the PLEGEN.DAT file for experienced users.

STATISTICS FOR MODEL EVALUATION

It is important to objectively judge whether a calibration or validation is satisfactory. Due to the complex and empirical nature of agricultural models, it is rare for a model to provide the same level of accuracy in simulating all system components. For example, one set of calibrated parameters may favor crop production over soil N simulation, and another may simulate soil water better than plant growth. Choosing one set of parameters over the other is mainly dependent on the user's objective and experiences. It is recommended to select a set of parameters that provide reasonable simulation results for all system components, not only those having measured data. In other words, users need to check all system outputs, not just the ones with corresponding field measurements, so that a good calibration of one system component is not achieved at the expense of the other (in other words, a good result is not obtained for the wrong reason). For example, crop yield may be simulated acceptably compared to field measurements, but simulated evapotranspiration or soil water content may be unrealistic.

Statistically, the unbiased root mean squared deviation (RMSD) or relative RMSD (RRMSD) should be used to determine goodness-of-calibration for each variable of interest (Fox, 1981):

$$\mathrm{RMSD} = \sqrt{\frac{\sum_{i=1}^{N}\left(P_i - O_i\right)^2}{N}} \tag{1}$$

$$\mathrm{RRMSD} = \frac{\mathrm{RMSD}}{\bar{O}} \tag{2}$$

where P_i and O_i are the model-predicted and experimentally measured (observed) points, respectively, N is the number of observations, and $\bar{O}$ is the averaged observed value. Percentage bias (PBIAS) is another statistic used commonly in model evaluation:

$$\mathrm{PBIAS} = \frac{\sum_{i=1}^{N}\left(P_i - O_i\right)\times 100}{\sum_{i=1}^{N}\left(O_i\right)} \tag{3}$$

Linear regression (r^2) should only be used for trend analysis because it can be biased:

$$r^2 = \frac{\left[\sum_{i=1}^{N}\left(O_i - \bar{O}\right)\left(P_i - \bar{P}\right)\right]^2}{\sum_{i=1}^{N}\left(O_i - \bar{O}\right)^2 \sum_{i=1}^{N}\left(P_i - \bar{P}\right)^2} \tag{4}$$

where $\bar{P}$ is the average of all predictions. Other statistics used mostly for water-related simulations are Nash-Sutcliffe model efficiency (NSE) (Nash and Sutcliffe, 1970) and D-index (Willmott, 1981):

$$\mathrm{NSE} = 1.0 - \frac{\sum_{i=1}^{N}\left(O_i - P_i\right)^2}{\sum_{i=1}^{N}\left(O_i - \bar{O}\right)^2} \tag{5}$$

$$\mathrm{D} = 1.0 - \frac{\sum_{i=1}^{N}\left(O_i - P_i\right)^2}{\sum_{i=1}^{N}\left(\left|P_i - \bar{O}\right| + \left|O_i - \bar{O}\right|\right)^2} \tag{6}$$

The advantage of using NSE and D is that a value of 1.0 indicates perfect calibration. As their values move away from 1.0, model calibration becomes worse. L. Ma et al. (2011) suggested NSE > 0.7, D > 0.7, $r^2 > 0.80$, and -15% < PBIAS < 15% as acceptable model simulation statistics based on the literature. A list of statistics is available from L. Ma et al. (2011). Another test that has not been used widely is the lack-of-fit test (LOFIT), which is an F-test that takes into account experimental errors among replicates (Whitmore, 1991; Roloff et al., 1998; Kersebaum et al., 2008) (see Appendix B). Paired t-test may be used in some cases (L. Ma et al., 1999).

CASE STUDY 1: IRRIGATED MAIZE IN COLORADO

A field experiment was initiated in 2008 near Greeley, Colorado (40.45° N, 104.64° W). The site contains three soil types, Nunn (fine, smectitic, mesic Aridic Argiustolls), Olney (fine-loamy, mixed, superactive, mesic Ustic Haplargids), and Otero (coarse-loamy, mixed, superactive, calcareous, mesic Aridic Ustorthents). The soil is a sandy loam and is fairly uniform throughout the 200 cm soil profile. Weather data were recorded on site with a standard Colorado Agricultural Meteorological Network (http://ccc.atmos.colostate.edu/~coagmet) weather station (GLY04). Missing data at the beginning of the study were estimated with data from a nearby station 800 m to the east (GLY03). The field was divided into 9 m × 44 m plots.

Maize (*Zea mays* L., variety Dekalb 52-59) was planted at an average rate of 81,000 seeds ha^{-1} with 0.76 m row spacing on 12 May 2008, 11 May 2009, and 11 May 2010 and harvested on 6 November 2008, 12 November 2009, and 19 October 2010. Four replicates were arranged by

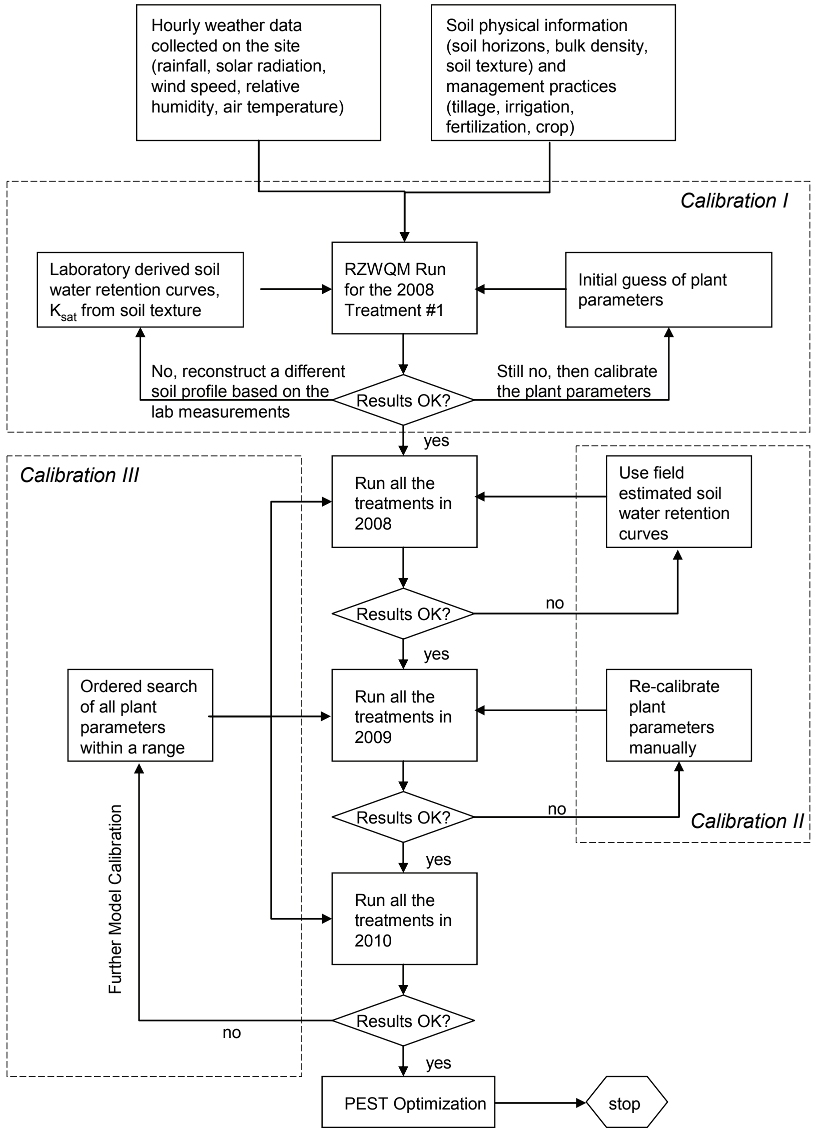

Figure 1. Calibration procedure for RZWQM2 in the Colorado study (adapted from L. Ma et al., 2012).

randomized complete block design. Five irrigation treatments (micro-irrigation with surface drip tubing adjacent to each row) within each replicate were designed to meet a certain percentage of potential crop ET (ET_c) requirements during the growing seasons: 100% (treatment 1), 85% (treatment 2), 70% (treatment 3), 55% (treatment 4), and 40% (treatment 5) of ET_c. Fertilizer as urea ammonium nitrate (UAN) was applied at planting and then with irrigation water during the growing seasons as needed based on estimated plant growth and possible N uptake. Total N applied was 134 kg N ha^{-1} in 2008, 160 kg N ha^{-1} in 2009, and 146 kg N ha^{-1} in 2010 for all treatments. Total irrigation amounts were 46.9, 36.9, 30.3, 21.1, and 16.7 cm in 2008; 41.7, 34.6, 24.9, 16.7, and 10.9 cm in 2009; and 36.5, 30.3, 21.9, 15.3, and 10.0 cm in 2010 for treatments 1 through 5, respectively (L. Ma et al., 2012).

MANUAL CALIBRATION AND GRID SEARCH

The objective of this case study was to investigate maize response to irrigation scheduling to meet different levels of crop evapotranspiration (ET_c) demand (L. Ma et al., 2012). Therefore, calibration was focused mainly on soil water content and crop production. Following the guidelines outlined earlier, the model was initially parameterized with laboratory-measured soil water retention curves (SWRCs) for different soil depths along with the texture-based K_{sat}, and then the plant parameters were manually calibrated for the least water-stressed treatment (treatment 1; 100% ET met) (fig. 1) (calibration I). Simulated yield for this treatment in 2008 was 11,059 kg ha^{-1} versus 11,071 kg ha^{-1} measured, and simulated harvest biomass was 21,487 kg ha^{-1} versus 22,112 kg ha^{-1} measured. Simulated anthesis day was 85 days after planting (DAP), and simulated physiological maturity date was 142 DAP, which were the same as the observed dates in the field. Simulated maximum leaf area index (LAI) was 4.80 versus 4.61 measured. There was no water stress simulated, as expected, but the model began to predict N stress in early September. Simulated RMSD was 0.778 for LAI, 0.039 cm^3 cm^{-3} for soil water contents, and 3.20 cm for the total soil profile water storage.

Table 7. Soil parameters estimated from field-measured soil water contents and from PEST optimization in the Colorado study (from L. Ma et al., 2012).

	Soil Depth (cm)	Sat. Hydraulic Conductivity (cm h^{-1})	θ_s (cm^3 cm^{-3})	$\theta_{1/3}$ (cm^3 cm^{-3})	θ_{15} (cm^3 cm^{-3})	h_b (cm)	λ (dimensionless)
Soil parameters estimated from field-measured soil water contents	0-15	6.11	0.437	0.262	0.131	20.04	0.182
	15-30	6.11	0.437	0.249	0.124	15.15	0.182
	30-60	6.11	0.437	0.220	0.110	7.75	0.182
	60-90	6.11	0.408	0.187	0.093	4.64	0.182
	90-120	6.11	0.408	0.173	0.086	2.95	0.182
	120-150	6.11	0.390	0.162	0.081	2.71	0.182
	150-200	6.11	0.390	0.198	0.099	8.04	0.182
Soil parameters optimized with PEST	0-15	10.00	0.437	0.254	0.125	18.16	0.186
	15-30	8.79	0.437	0.240	0.107	20.00	0.212
	30-60	10.00	0.437	0.235	0.120	10.00	0.177
	60-90	10.00	0.408	0.200	0.103	5.69	0.174
	90-120	10.00	0.408	0.196	0.111	4.12	0.150
	120-150	10.00	0.390	0.191	0.108	5.00	0.150
	150-200	8.20	0.390	0.213	0.120	15.00	0.150

Table 8. Plant parameters calibrated for maize in the study using soil water retention curves from estimated field capacity in the Colorado study (from L. Ma et al., 2012).

		Grid Search of Plant Parameters		PEST Optimization Range	
	Abbreviations and Definitions of Traits	Range Searched	Selected Value	Range to Optimize	Optimized Value
P1	Degree days (base temperature of 8°C) from seedling emergence to end of juvenile phase (thermal degree days).	250-290, increment of 10	260	250-290	251
P2	Day length sensitivity coefficient, the extent (days) that development is delayed for each hour increase in photoperiod above the longest photoperiod (12.5 h) at which development proceeds at maximum rate.	0.2-0.6, increment of 0.2	0.2	0.2-0.6	0.27
P5	Degree days (base temperature of 8°C) from silking to physiological maturity (thermal degree days).	550-620, increment of 10	570	550-620	620
G2	Potential kernel number.	900-1000, increment of 20	920	900-1000	991
G3	Potential kernel growth rate (mg per kernel per day).	5-10, increment of 1	7	5-10	6.3
PHINT	Degree days required for a leaf tip to emerge (phylochron interval) (thermal degree days).	35-55, increment of 5	50	35-5 5	49.6

After calibration, the model was used to simulate other irrigation treatments in 2008. Simulated yield and biomass did not respond to irrigation treatments. As a result, we used estimated field capacity (FC) in the field after a big storm as soil water content at 33 kPa (table 7). Using the same plant parameters as calibrated above, we simulated yield and biomass for the 100% ET treatment in 2008 within 10% of measured values (10,073 kg ha^{-1} vs. 11,071 kg ha^{-1} for yield, and 20,014 kg ha^{-1} vs. 22,112 kg ha^{-1} for biomass) and matched both anthesis and physiological maturity dates well (85 vs. 85 DAP for anthesis and 144 vs. 142 DAP for maturity). However, the model still did not respond to irrigation in 2009. The simulated anthesis date was 99 DAP compared to the observed 85 DAP in 2009.

Therefore, we recalibrated the plant parameters (calibration II, fig. 1) to make sure the anthesis dates were reasonable for both 2008 and 2009 and increased the yield and biomass responses to irrigation in 2008 by increasing the kernel number and decreasing the grain filling rate. We also found that reducing the day length sensitivity coefficient improved biomass simulation. In addition, we used the default 38.9°C-d phylochron interval (PHINT; see plant parameters in table 8). These parameters improved yield and biomass responses to irrigation amounts. The RMSD across all five treatments were 0.037 cm^3 cm^{-3} for soil water content and 3.9 cm for profile soil water for 2008 (table 9). Although the maximum LAI simulated for treatment 1 was close to measured (4.5 compared to 4.6), the peak LAI was 10 days early compared to maximum canopy cover. Both simulated anthesis and maturity dates were also advanced by a week compared to observed dates.

For 2009, the simulated anthesis date was 85 compared to 84 DAP observed, and the maturity date was 143 compared to 147 DAP observed. The simulated RMSD was 387 kg ha^{-1} for yield and 1400 kg ha^{-1} for biomass. Simulated soil water content and profile soil water were slightly better than those for 2008, with RMSD of 0.030 cm^3 cm^{-3} and 2.4 cm, respectively. These calibrated parameters simulated maize yield well in 2010 for treatments 3, 4, and 5 but underpredicted yield for treatments 1 and 2, with an overall RMSD of 1722 kg ha^{-1}. On the contrary, the model predict-

Table 9. Simulated root mean squared deviation (RMSD) with RZWQM2 in the Colorado study.

	2008	2009	2010	Avg.
Grid search on plant and soil parameters from field-measured soil water content				
Yield (kg ha^{-1})	651	585	531	589
Biomass (kg ha^{-1})	1594	1044	2776	1804
LAI	0.93	0.98	0.69	0.87
Soil water content (cm^3 cm^{-3})	0.037	0.030	0.056	0.041
Soil water storage (cm)	3.93	2.38	3.17	3.16
Soil and plant parameters optimized with PEST				
Yield (kg ha^{-1})	388	498	618	501
Biomass (kg ha^{-1})	1136	1200	1677	1337
LAI	1.02	0.91	0.58	0.84
Soil water content (cm^3 cm^{-3})	0.035	0.027	0.046	0.036
Soil water storage (cm)	3.59	2.22	3.12	2.98

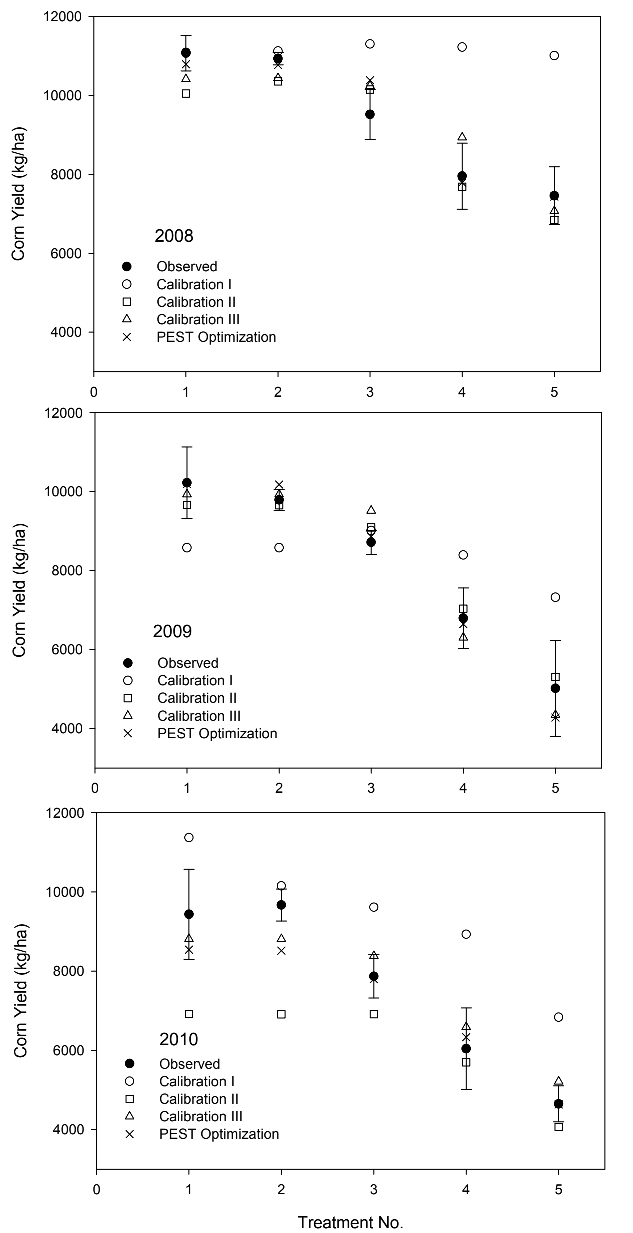

Figure 2. Step-by-step calibration of maize yield in the Colorado study based on calibration procedure outlined in figure 1. Detail calibration procedure and data are available from L. Ma et al. (2012).

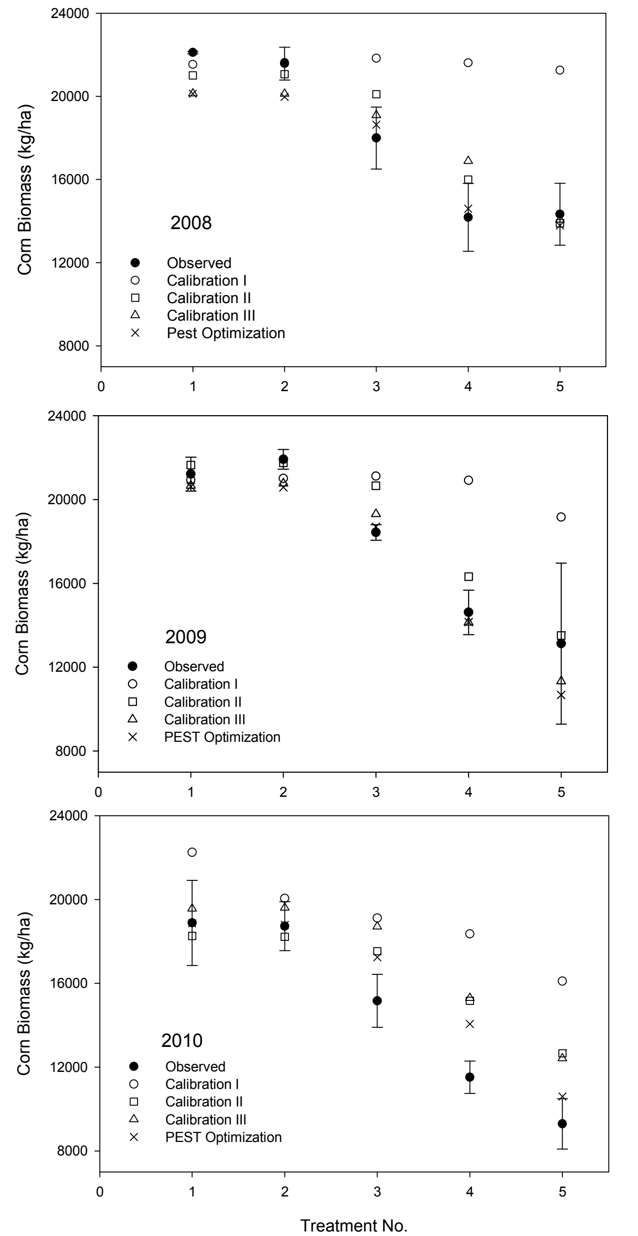

Figure 3. Step-by-step calibration of maize biomass in the Colorado study based on calibration procedure outlined in figure 1. Detail calibration procedure and data are available from L. Ma et al. (2012).

ed biomass well in 2010 for treatments 1 and 2 but considerably overpredicted biomass for the other treatments, with overall RMSD of 2439 kg ha^{-1}. Therefore, we conducted a grid search of the plant parameters within a certain range (calibration III, fig. 1) to see whether we could improve the 2010 simulation results while maintaining the good prediction for 2008 and 2009 (table 8). The range for each parameter was derived from the plant parameter database in DSSAT. A total of 14,068 model runs were executed. As a result, we selected one set of plant parameters that improved simulation for all three years (tables 9; figs. 2 and 3). However, biomass was still not simulated as well as expected, especially in 2010.

AUTOMATED CALIBRATION WITH PEST

We used PEST to further calibrate the model to see whether additional improvement could be made using the method outlined by Nolan et al. (2011). Here, the Brooks-Corey parameters were optimized through the pore size distribution index (λ) and bubbling pressure (h_b), with λ ranging from 0.15 to 0.25 and h_b varying 50% above and below its original values for each soil layer. Saturated soil hydraulic conductivity (K_{sat}) was optimized within the range of 1 to 10 cm h^{-1}. Plant parameters were optimized within the same ranges as in the ordered search above (L. Ma et al., 2012; table 8).

An overall objective function was defined in the following form:

$$\Phi = \sum_{i=1}^{n} \sum_{j=1}^{m_i} w_i^2 \left(y_{i,j} - y'_{i,j} \right)^2 \tag{7}$$

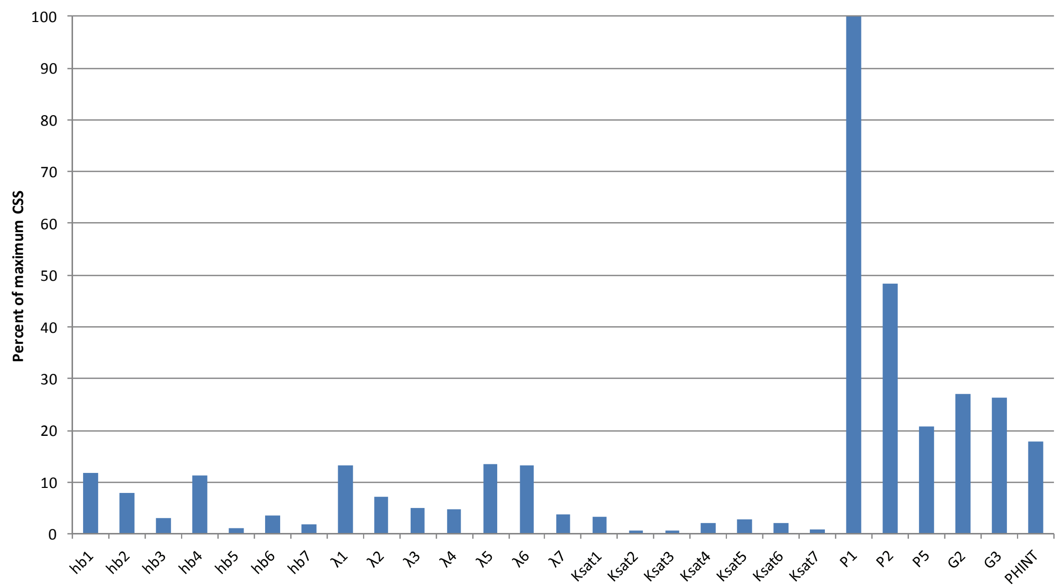

Figure 4. Normalized composite scaled sensitivity (CSS) of RZWQM2 parameters adjusted by PEST in the Colorado study. Numbers on the *x*-axis labels for the soil parameters indicate soil horizon layers 1 through 7. See Appendix A for the Brooks-Corey parameter definitions of h_b, λ, and K_{sat} and table 8 for definitions of plant parameters P1, P2, P5, G2, G3, and PHINT.

where n is the number of output variables to optimize, m_i is the number of observations for each variable, w_i is the assigned weight for each observation, and $y_{i,j}$ and $y'_{i,j}$ are paired observed and simulated values. In this study, five output variables were included in the Φ value: maize yield, maize biomass, LAI, soil water content, and soil water storage in the soil profile, with weights of 0.05, 0.02, 8, 75, and 2, respectively. These weights were initially determined using an error-based approach (Hill and Tiedeman, 2007) as the inverse of the standard deviation of each group of observations, and then adjusted such that no observation group dominated or was dominated by the other groups. The end result was that the five observation groups (output variables) had about the same sum of squares contribution to the objective function (Φ) value.

We used truncated singular value decomposition (SVD) to mitigate potential problems with parameter interdependence and insensitivity. This method is a "subspace method" that estimates linear combinations (SVD parameters) of the original process model parameters (Doherty and Hunt, 2010). The SVD parameters are by definition uncorrelated and, through truncation, only the most sensitive SVD parameters are estimated.

The optimization started with parameters from the ordered search of plant parameters, field-estimated SWRCs, and texture-based K_{sat} values with an initial Φ value of 112,552. After 14 iterations and 744 model runs, the Φ value was reduced by 29% to 79,808. Although the optimized plant and soil parameters are only slightly different from their initial values (tables 7 and 8), PEST improved overall

Table 10. Final statistics after PEST optimization for simulated corn grain yield and biomass in the Colorado study for the five irrigation treatments in 2008, 2009, and 2010, and soil water content for the 100% ET treatments in 2008 only: RMSD = root mean squared deviation, RRMSD = relative RMSD, r^2 = coefficient of determination, NSE = Nash-Sutcliffe model efficient, D = D-index of agreement, RS_pR = RMSD to S_p ratio (see Appendix B), and F(LOFIT) = F-value for the lack-of-fit test.

Simulated Variable	Year	RMSD	RRMSD	r^2	NSE	D	RS_pR	LOFIT (one-tail) F-Value	LOFIT (one-tail) p-Value
Yield	2008	422	0.045	0.922	0.919	0.980	0.691	1.911	0.152
	2009	384	0.047	0.993	0.961	0.992	0.493	0.973	0.465
	2010	665	0.088	0.962	0.882	0.963	0.855	2.923	0.048
	All years	506	0.061	0.941	0.933	0.983	0.696	1.937	0.044
Biomass	2008	1213	0.067	0.934	0.873	0.960	0.976	3.811	0.020
	2009	1295	0.073	0.952	0.862	0.970	0.704	1.985	0.139
	2010	1581	0.107	0.947	0.829	0.949	1.170	5.477	0.005
	All years	1372	0.081	0.881	0.875	0.963	0.914	3.347	<0.001
Soil water content (2008 only)	0-15 cm	0.047	0.234	0.440	-0.083	0.792	2.713	29.433	<0.001
	15-30 cm	0.036	0.162	0.492	-0.334	0.785	1.530	9.365	<0.001
	30-60 cm	0.025	0.119	0.600	-1.079	0.754	0.336	0.451	0.984
	60-90 cm	0.024	0.128	0.416	-0.491	0.740	0.358	0.512	0.966
	90-120 cm	0.032	0.195	0.349	-2.471	0.617	0.391	0.611	0.911
	120-150 cm	0.015	0.105	0.636	0.313	0.869	0.259	0.267	0.999
	150-200 cm	0.007	0.039	0.922	0.775	0.953	0.397	0.634	0.894
	All layers	0.029	0.155	0.480	0.351	0.774	0.516	1.065	0.313
Total water storage (cm)		4.34	0.136	0.833	0.773	0.797	0.507	1.030	0.442

simulation results for all three years for both plant growth and soil water content (tables 9; figs. 2 and 3). Because PEST is a local estimation method, the number of runs was much less than with the grid search method (L. Ma et al., 2012), which focused only on plant parameters.

Composite scaled sensitivities (CSS) computed on the basis of the original process model parameters are shown in figure 4. CSS shows the total amount of information provided by the observations for estimation of a single parameter (Hill and Tiedman, 2007). In the figure, the CSS values are normalized to the maximum CSS and expressed in percent. The CSS values indicate that plant parameters are more important than the other parameters based on this dataset. Three of the process-model parameters are difficult to estimate ($K_{sat}2$, $K_{sat}3$, $K_{sat}7$) according to CSS. This is not critical, because we used SVD to estimate SVD parameters (CSS is related to the singular vectors and singular values used in SVD, but pertains to the original process model parameters).

After further calibration with PEST, biomass simulation was much improved (figs. 2 and 3) in terms of RMSD. Simulated yield was improved in 2008 and 2009 but became a little worse in 2010, although overall prediction of yield across the three years was improved. Improvement to soil water simulation was minor if any. However, optimized results may change if different weights were used. Table 10 lists other statistics after the PEST optimization. For yield and biomass, the D-index and NSE were high (>0.80), and

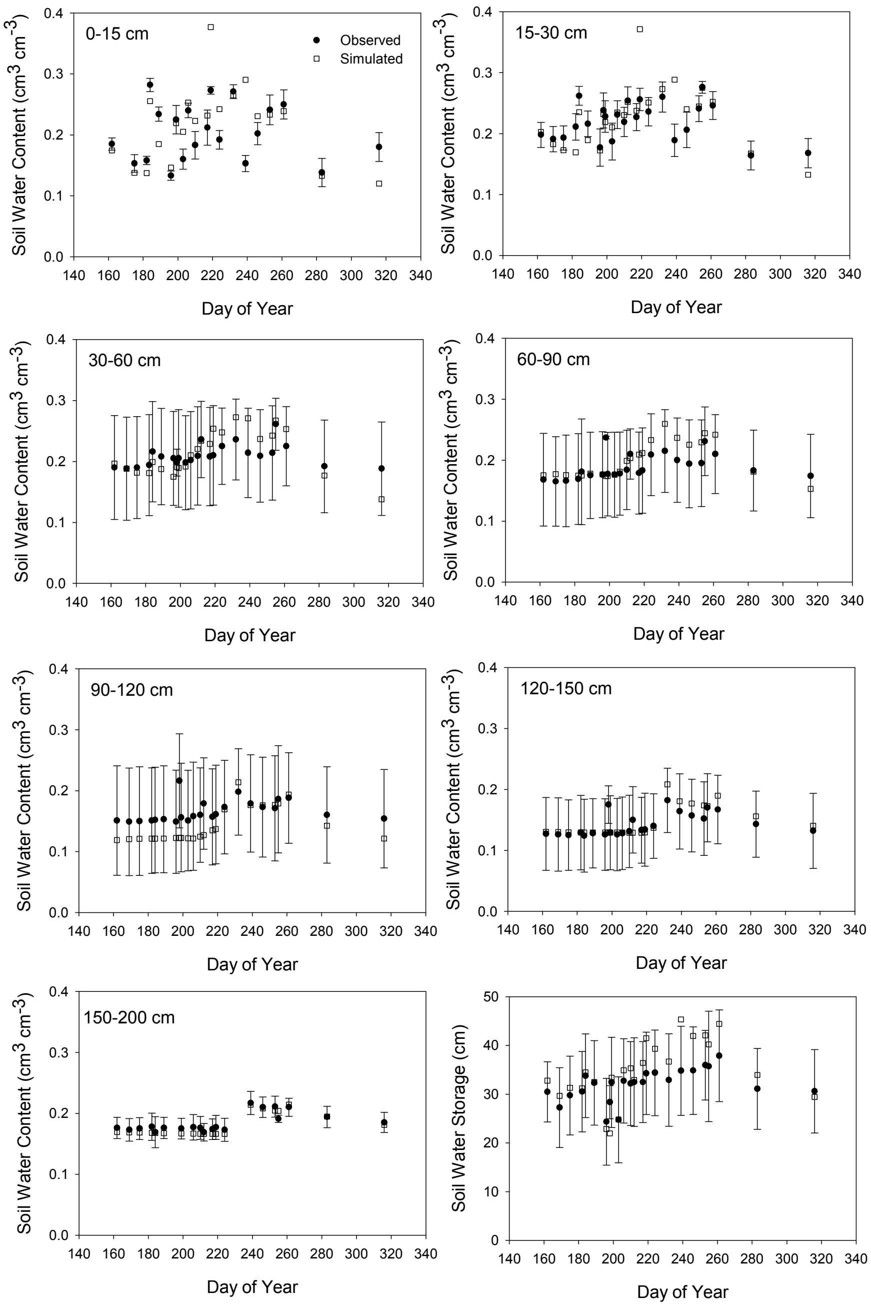

Figure 5. Measured and simulated soil water content for the 100% ET$_c$ treatment in 2008 in the Colorado study. Detail calibration procedures and data are available from L. Ma et al. (2012).

the RRMSD was under 10%. However, the LOFIT test showed that at the 0.05 level of significance ($\alpha = 0.05$), only yields in 2008 and 2009 were acceptable and only 2009 biomass was acceptable. If the level of significance was reduced to 0.01 ($\alpha = 0.01$), biomass simulation in 2010 was still not acceptable. For simulation of soil water content of treatment 1 in 2008, the D-index was greater than 0.60, but NSE was less than zero and r^2 was less than 0.6 for the top five soil horizons, which suggests that a mean soil water content was better than the RZWQM2 simulations. However, based on the LOFIT test, soil water content simulation was acceptable due to large experimental error (fig. 5), but it would be difficult to make a conclusive evaluation of the model performance when NSE < 0. When NSE > 0, the results in table 10 suggest that model simulation is very good when $p > 0.10$, good if $p > 0.05$, and satisfactory if $p > 0.01$. The statistical analyses also show that high NSE may be obtained when there is a large variability in the measured results, as in the cases of yield and biomass (ranging from 5,000 to 11,000 kg ha^{-1} for yield and from 9,000 to 22,000 kg ha^{-1} for biomass among the five irrigation treatments) due to the calculated deviation of O_i from the overall mean ($\overline{O}$) in equation 5. It is also interesting to note that $RS_pR < 0.8$ corresponds to $p > 0.05$ and $RS_pR < 1.0$ corresponds to $p > 0.01$ of the LOFIT test (table 10).

Case Study 2: Maize-Soybean and Cover Crop under Subsurface Drainage in Iowa

The objective of this field experiment was to investigate winter rye cover crop impacts on subsurface drainage, NO_3-N loss, and maize and soybean yield in a subsurface drained field in subhumid Iowa. Field plots were located at the Agricultural Drainage Water Quality Research and Demonstration Site near Gilmore City, Iowa (42.75° N, 94.50° W), operated by Iowa State University. Predominant soils are Nicollet (fine-loamy, mixed, superactive, mesic Aquic Hapludoll), Canisteo (find-loamy, mixed, superactive, calcareous, mesic Typic Endoaquolls), and Okoboji (fine, smectitic, mesic Cumulic Vertic Endoaquolls). The 78 plots were grouped into four blocks by drainage characteristics based on the long-term drainage performance. Land cover treatments in this study were: winter rye growth prior to maize in odd years and prior to soybean in even years (TRT1), winter rye cover crop growth prior to soybean in odd years and prior to maize in even years (TRT2), maize in odd years and soybean in even years without cover crop (CTRL1), and soybean in odd years and maize in even years without cover crop (CTRL2).

The experimental phase that included winter cover crop for maize and soybean (TRT1 and TRT2) was initiated in October 2004 by planting rye as a winter cover crop after maize and soybean harvest. In subsequent years, a winter rye cover crop continued to be planted after maize and soybean within the commonly adopted maize-soybean rotation cropping system in Iowa. Rye was killed by glyphosate in the following April or May, and planting dates were in early to mid-May for maize and late May for soybean. Aqueous ammonia-nitrogen was applied at 140 kg N ha^{-1} to maize in spring after maize emergence. Data collected in this study included weather information, soil physical properties, soil water content, subsurface drainage flow, and NO_3-N concentration in the drainage, crop total aboveground biomass and yield, and plant N uptake. This experiment lasted five years (2005 to 2009), and detailed field management activity and timing since October 2004 are provided by Qi et al. (2011).

Model Calibration

First, a quality check of observed data was conducted prior to running the model. The weather station tended to be affected by thunderstorms. Missing values of weather information were filled using data from neighboring stations. Drainage flow data due to malfunction of the sump were discarded. Second, we identified experimentally measured data for drainage flow, soil water storage, NO_3-N loss in drainage, crop N uptake, total aboveground biomass, and grain yield for model parameterization using a trial-and-error method. The measured data had the same precision and the same spatial and temporal resolution for each plot. Experimental measurements from TRT1 from 2005 to 2009 were selected as the calibration dataset and the other three treatments (CTRL1, TRT2, and CTRL2) were used to validate the RZWQM2 model.

Model calibration was conducted in the order of water, nitrogen, and crop growth, and then iterated several times in that order. Soil physical and hydraulic properties such as SWRCs and saturated hydraulic conductivity (K_{sat}) were obtained by laboratory measurements for site-specific soil cores (Qi et al., 2011). Lateral hydraulic conductivity (LK_{sat}), which is a key parameter to calculate subsurface drainage flow in Hooghoudt's equation, was set to $2K_{sat}$ to match the peak of daily drain flow. To get a better simulation of soil water storage, the soil root growth factor (SRGF) in the crop module was adjusted for maize, soybean, and rye. To improve biomass simulation, plant parameters related to leaf number and leaf area index were calibrated, which in turn affected soil moisture simulation. For nitrogen, the chemical background of precipitation was set to 0.5 mg N L^{-1} for NH_4-N and 1.3 mg N L^{-1} for NO_3-N according to the online information provided by the National Atmospheric Deposition Program (http://nadp.sws.uiuc.edu). The initial residual N in the soil profile, including crop residue, soil organic matter, microorganisms, and surface residue properties, was from Thorp et al. (2007) except that the death rate of aerobic heterotrophs was adjusted from 9×10^{-37} to 4×10^{-37} to match the NO_3-N concentration in the drainage.

Crop parameters for maize (IB 1068 Dekalb 521) and soybean (990002 M Group 2) were essentially default values with minor modification. For maize, the phylochron interval between successive leaf tip appearances (PHINT) was adjusted to obtain harvest indices around 0.50. The PHINT value was modified within the range between 60 (Thorp et al., 2007) and 38.9 (L. Ma et al., 2006), and a value of 40 was selected to simulate aboveground biomass

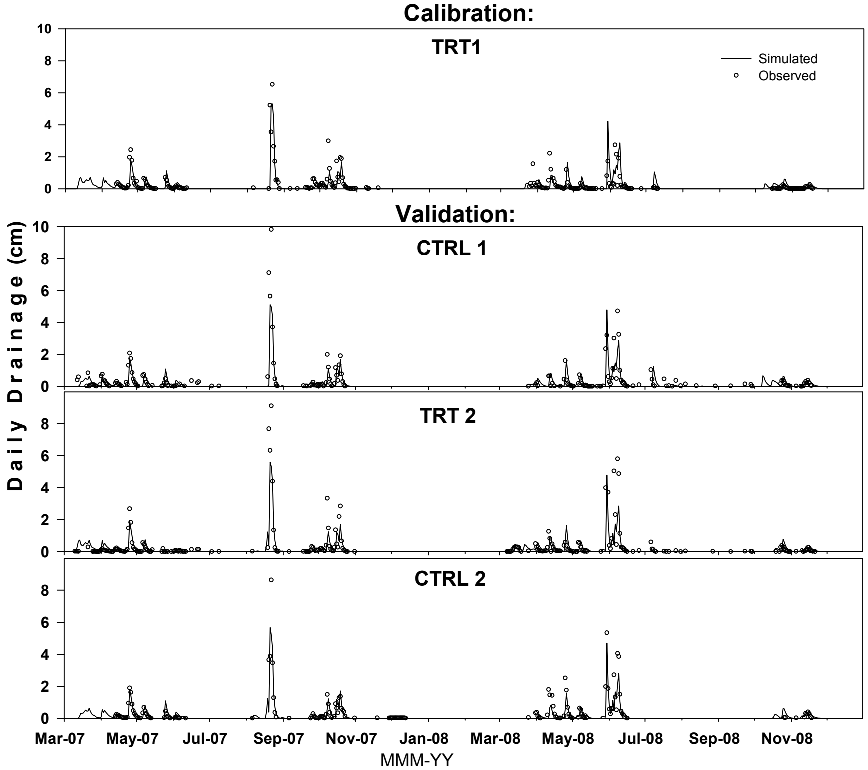

Figure 6. Observed and simulated daily drainage in 2007 and 2008 (from Qi et al., 2011).

accumulation. Kernel number (G2) and grain fill (G3) parameters were adjusted to 750 and 6.75, respectively, to improve yield simulation. For soybean, LFMAX (maximum leaf photosynthesis rate) was adjusted to 0.97 (mg CO_2 $m^{-2}s^{-1}$) for better yield simulation. For winter rye, attention was paid to parameters related to emergence and leaf growth. In order to reduce the overestimation of biomass of winter rye in the early stage before late April in each year, the emergence phase duration (PECM) and the germination phase duration (PEG) were set to 25 and 75°C-d, respectively, similar to the values calibrated by Thorp et al. (2010). The area of standard leaf and lamina leaf area to weight ratio were adjusted to improve leaf area index simulation in 2007 and 2008.

After the iterative calibration, the total annual drainage in 2005-2009 for the calibration treatment (TRT1) was simulated with NSE equal to 0.88. Simulated and observed daily drain flow in 2007 and 2008 are shown in figure 6. The NSE and PBIAS values for the daily drain flow simulation in the calibration treatment (TRT1) were 0.50 and 7%. The RMSD value for soil water storage in TRT1 was 1.0 cm, which was 5% of the average measured values (fig. 7). Annual NO_3-N

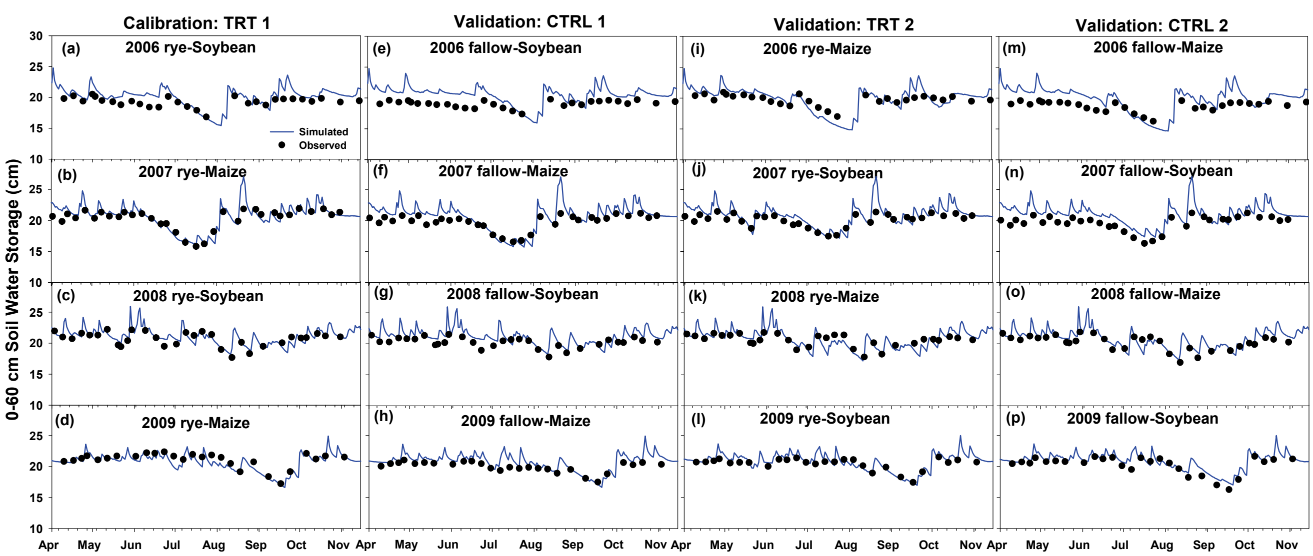

Figure 7. Average measured and simulated soil water storage in the 0-60 cm profile in the (a-d) calibration plots of TRT1, and validation plots of (e-h) CTRL1, (i-l) TRT2, and (m-p) CTRL2 in the Iowa study (from Qi et al., 2011).

Table 11. Soil water balance (cm) for the four treatments (TRT1, CTRL1, TRT2, CTRL2) in Iowa from 2005 to 2009.

Treatment	Precip-itation	ET	Tile Drainage	Runoff	Change in Soil Water Storage	Water Balance Error[a]
TRT1	82.6	45.6	31.5	4.8	1.4	-0.7
CTRL1	82.6	44.9	32.3	4.8	1.4	-0.6
TRT2	82.6	44.1	32.9	4.8	1.4	-0.5
CTRL2	82.6	45.9	31.2	4.7	1.4	-0.6
Average	82.6	45.2	32.0	4.8	1.4	-0.6

[a] Water balance error = input – output.

loss in drain flow was simulated with NSE equal to 0.84 for TRT1 and RMSD of 6.57 kg N ha^{-1}. Simulated aboveground N uptake by maize and soybean were within ±11% error with RRMSD of 16%. The time series data of rye N uptake was predicted with an NSE value of 0.74 for TRT1. The RRMSD value was within 21% for maize and soybean yield and within 18% for total aboveground biomass of maize and soybean. The RRMSD value was within 11% for rye biomass simulation.

MODEL VALIDATION

For the validation treatments (CTRL1, TRT2, and CTRL2), annual tile drainage in 2005-2009 was simulated with NSE values of 0.91, 0.84, and 0.40, respectively. The 24% overestimation in drainage for CTRL2 might be attributed to water loss through lateral seepage. Soil water storage was simulated with RMSD ranging from 1.0 to 1.4 cm, less than 7% of the observed average for each validation treatment (fig. 7). Annual NO_3-N loss in drain flow for CTRL1, TRT2, and CTRL2 was simulated with NSE values of 0.73, 0.74, and 0.46, respectively. The overestimation of 16% in NO_3-N loss in CTRL2 was a result of overestimated drain flow. Simulated aboveground N uptake by maize and soybean were within ±7% error with RRMSD ≤ 24%. For TRT2, simulated rye N uptake was overestimated by 22% with NSE of only 0.03. This overestimation mainly occurred in 2009. When excluding 2009 data, the NSE value increased to 0.68. The RRMSD values for maize and soybean yield simulation were within 19%, 10%, and 12% error for CTRL1, TRT2, and CTRL2, respectively. Maize biomass was simulated within 5% error and with RRMSD equal to 25%. Soybean biomass was generally overestimated by 41% for the validation plots. Rye biomass in TRT2 was simulated within 12% error and with RRMSD equal to 28%.

MASS BALANCE

For any simulation, it is important to check processes that have no measurement data. Table 11 lists water balance and table 12 lists nitrogen balance for the Iowa study. Although ET was not measured in the study, simulated ET was reasonable compared to a study in Iowa by Jaynes and Miller (1999). For N balance, the annual mineralization was not measured either, but the simulated values are reasonable within the range given by Schepers and Mosier (1991), although it is on the high side. N fixation was within the range give by Schepers and Mosier (1991). Immobilization

Table 12. Soil nitrogen balance (kg N ha^{-1}) in the Iowa study for the four treatments (TRT1, CTRL1, TRT2, CTRL2) from 2005 to 2009.

N Components		TRT1	CTRL1	TRT2	CTRL2
Inorganic N in the soil profile					
	Initial value	200.9	199.0	197.2	204.0
	Ending value	196.2	194.6	192.8	199.8
Gain	Rain water	13	13	8	13
	Fertilization	84	84	56	56
	Mineralization	180	159	175	159
	Fixation	88	82	144	133
Losses	Denitrification	4	3	3	3
	Volatilization	0	0	0	0
	Runoff	0	0	0	0
	Deep seepage	0	0	0	0
	Tile drainage	36	42	33	39
	Lateral flow	0	0	0	0
	Plant uptake	311	277	336	304
	Immobilization	18	19	16	19
N balance error[a]		-0.01	0.12	0.33	0.35

[a] N balance error = gain – losses + change in soil N.

of inorganic N to microbial biomass was between 16 and 19 kg N ha^{-1} year^{-1}, which is reasonable. Low values of simulated denitrification, volatilization, runoff, and seepage were expected for the tile-drained soil with fertilizer injection. Therefore, the calibration results were obtained for the right reasons.

DISCUSSION

RZWQM2 is a one-dimensional, point-scale model, so it should be used only for an average field condition. Where there is obvious heterogeneity in the field, the model should be used either by simulating each subunit or by using average soil inputs. Due to the one-dimensionality, runoff and runon are not simulated for each subunit. In addition, water detention due to surface roughness is not simulated, neither are ponding infiltration and interception of rainfall by crop canopy and residue (in the current released version). Although the model contains a soil equilibrium chemistry module to simulate ion exchange and changes in soil pH and salinity, it has not been fully evaluated. The use of the Richards equation for water redistribution can occasionally cause non-convergence problems when there are abrupt changes in soil hydraulic properties in the soil profile. Another weakness of the model is that it cannot simulate intercropping (growing two crops at the same time).

With the incorporation of the DSSAT crop growth model and the SHAW model, RZWQM2 has become one of the most comprehensive system models. Therefore, it is applicable to a wide range of soil, weather, and management conditions. The development of a Windows-based user interface has helped model application tremendously (L. Ma et al., 2000a, 2007d). RZWQM2 is one of the few models that simulates pesticide uptake by plants, equilibrium and kinetic adsorption, degradation and irreversible adsorption, volatilization, and macropore transport of pesticides. Chemical loss in runoff water is also a unique feature of RZWQM2. The model's ability to simulate subsurface (tile) drainage, water table fluctuation, and agricultural nutrient losses in tile flow is also a plus for water quality simulation in drained soils (Qi et al., 2011; L. Ma et al., 2007a, 2007b, 2007c). The inclusion of many management practices (tillage, irrigation, fertilization, crop rotation, and manure application) makes RZWQM2 unique for many agricultural applications. Its ability to simulate microbial growth and death is a desirable feature for studying soil organic carbon/nitrogen cycling. The use of RZWQM2 to run crop rotation sequences over long periods of time is also widely recognized in the literature, especially under projected climate change conditions.

Future Developments

To overcome the weakness as a one-dimensional model, a prototype RZWQM2 and GIS linkage is being developed. New effort is underway to develop an erosion component for RZWQM2. Another major effort is to automate PEST application for model parameterization in RZWQM2. Efforts are also under consideration to add greenhouse gas (GHG) simulation, interception of rainfall by crop canopy and residue, and the effect of surface roughness on runoff and ponding infiltration and improve plant water stress simulations based on surface (canopy and soil) energy balance. Adding phosphorus to the model is under consideration, especially for soil water quality applications along with soil erosion. Finally, extending the model to flooded soil conditions (e.g., rice paddy) is also a future goal for the RZWQM2 team.

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APPENDIX A: THE BROOKS-COREY EQUATIONS

The modified Brooks-Corey equations used in RZWQM2 to describe soil water retention curves (Brooks and Corey, 1964; Ahuja et al., 2000b) are as follows:

$$\begin{aligned} \theta &= \theta_s + ah \qquad \text{when } |h| < |h_b| \\ \theta - \theta_r &= B \times |h|^{-\lambda} \qquad \text{when } |h| \geq |h_b| \end{aligned} \tag{A-1}$$

where θ_s and θ_r are saturated and residual soil water contents (cm^3 cm^{-3}), h_b is the air entry water suction for the soil water content (θ) and soil water suction (h) curve (cm), a is a constant (zero in most cases), and λ is the slope of the log(θ) and log(h) curve (dimensionless) and is also called pore size distribution index. By imposing continuity at h_b, $B = (\theta_s - \theta_r) \times h_b^{\lambda}$. The unsaturated hydraulic conductivity versus suction head, $K(h)$, is related as:

$$\begin{aligned} K(h) &= K_{sat} h^{-N_1} \qquad \text{when } |h| < |h_{bk}| \\ K(h) &= C_2 |h|^{-N_2} \qquad \text{when } |h| \geq |h_{bk}| \end{aligned} \tag{A-2}$$

where K_{sat} is the saturated hydraulic conductivity (h = 0) (cm h^{-1}), N_1 is a constant (zero in most cases), h_{bk} is the air entry water suction for the soil hydraulic conductivity (K) and suction head (h) curve (cm), and N_2 is the slope of the log(K) and log(h) curve. C_2 is obtained by imposing continuity at h_{bk}:

$$C_2 = K_{sat} \times h_{bk}{}^{N_2 - N_1} \tag{A-3}$$

N_2 in RZWQM2 is calculated as:

$$N_2 = 2 + 3 \times \lambda \tag{A-4}$$

The parameters h_b and h_{bk} are assumed to be equal, and θ_r is residual soil water content for a soil texture based on Rawls et al. (1982).

APPENDIX B: THE LACK-OF-FIT TEST (LOFIT)

For convenience, we first establish the following definitions:

N = number of experimental or measurement groups. The groups may represent different treatments or different sampling dates.

K_i = number of experimental replicates for the ith experimental or measurement group.

O_{ij} = jth observation (replicate) for the ith measurement group ($O_{ij} = \mu_i + \varepsilon_{ij}$ and $E[O_{ij}] = \mu_i$).

μ_i = true mean of observations for the ith experimental or measurement group.

$M = \sum_{i=1}^{N} K_i$ = total number of observations in the experiment.

P_i = predicted value for the ith experimental or measurement group based on a simulation model. P_i is treated as constant with no variance and is independent of O_{ij}.

$O_i = \frac{1}{K_i}\sum_{j=1}^{K_i} O_{ij}$ = mean of the ith experimental or measurement group.

$\bar{O} = \frac{1}{N}\sum_{i=1}^{N} O_i$ = grand experimental mean of the N groups.

$S_i^2 = \frac{1}{K_i - 1}\sum_{j=1}^{K_i}\left(O_{ij} - O_i\right)^2$ = sample variance of ith experimental or measurement group.

$S_p^2 = \frac{\sum_{i=1}^{N}(K_i - 1)S_i^2}{\sum_{i=1}^{N}(K_i - 1)}$ = pooled sample variance under equal variance assumption among the N groups.

For an experiment with N experimental or measurement groups and K_i replicates in each group, total sum of squared prediction errors (TSS) may be written as:

$$\text{TSS} = \sum_{i=1}^{N}\sum_{j=1}^{K_i}\left(P_i - O_{ij}\right)^2 \tag{B-1}$$

which can be rearranged as:

$$\begin{aligned}
\text{TSS} &= \sum_{i=1}^{N}\sum_{j=1}^{K_i}\left[\left(P_i - O_i\right) + \left(O_i - O_{ij}\right)\right]^2 \\
&= \sum_{i=1}^{N}\sum_{j=1}^{K_i}\left(P_i - O_i\right)^2 + \sum_{i=1}^{N}\sum_{j=1}^{K_i}\left(O_{ij} - O_i\right)^2 \\
&\quad + 2\sum_{i=1}^{N}\left(P_i - O_i\right)\sum_{j=1}^{K_i}\left(O_i - O_{ij}\right) \\
&= \sum_{i=1}^{N}\sum_{j=1}^{K_i}\left(P_i - O_i\right)^2 + \sum_{i=1}^{N}\sum_{j=1}^{K_i}\left(O_{ij} - O_i\right)^2 \\
&\quad + 2\sum_{i=1}^{N}\left(P_i - O_i\right)\left[K_i O_i - \sum_{j=1}^{K_i} O_{ij}\right] \\
&= \sum_{i=1}^{N}\sum_{j=1}^{K_i}\left(P_i - O_i\right)^2 + \sum_{i=1}^{N}\sum_{j=1}^{K_i}\left(O_{ij} - O_i\right)^2 \\
&= \sum_{i=1}^{N} K_i\left(P_i - O_i\right)^2 + \sum_{i=1}^{N}\sum_{j=1}^{K_i}\left(O_{ij} - O_i\right)^2 \\
&= \text{LOFIT+SSE}
\end{aligned} \tag{B-2}$$

where LOFIT is the sum of squared errors between predicted and observed mean values (due to lack-of-fit), and SSE is the sum of squared error due to experimental error (ε_{ij}). SSE may be rewritten as (Wackerly et al., 2008):

$$\text{SSE} = \sum_{i=1}^{N}\sum_{j=1}^{K_i}\left(O_{ij} - O_i\right)^2 = \sum_{i=1}^{N}(K_i - 1)S_i^2 \tag{B-3)}$$

The mean LOFIT (MSLOFIT) and mean SSE (MSE) are defined as:

$$\text{MSLOFIT} = \frac{\text{LOFIT}}{M}$$

$$\text{MSE} = \frac{\text{SSE}}{M - N} = \frac{\sum_{i=1}^{N}(K_i - 1)S_i^2}{\sum_{i=1}^{N}(K_i - 1)} = S_p^2 \tag{B-4}$$

Therefore, an F-test statistic can be constructed as (Kersebaum et al., 2008):

$$\text{F} = \frac{\text{MSLOFIT}}{\text{MSE}} \tag{B-5}$$

with degrees of freedom of $\nu_1 = M$ for the numerator and $\nu_2 = M - N$ for the denominator. To test whether model predic-tions (P_i) correctly estimate the true mean of the observa-tions for the ith experimental or measurement group, the hypothesis would be:

H_o: $P_i = \mu_i$ for all i

H_a: $P_i \neq \mu_i$ for at least one i

Rejection of H_o would indicate a "lack-of-fit" of the simulations with respect to the true experimental means. At a given level of significance (e.g., α level), a critical $F_{\alpha,\nu1,\nu2}$

value can be used to test the acceptability of the null hypothesis. If the calculated F-value does not exceed the critical F-value, then the null hypothesis is accepted. Otherwise, the null hypothesis is rejected, indicating a "lack-of-fit" of the simulation results to the observed means. Since the critical value of $F_{\alpha,\nu1,\nu2}$ increases with decreasing α level at the same degrees of freedoms (ν_1 and ν_2), the null hypothesis may be rejected more easily at high α level. Therefore, the null hypothesis rejected at α = 0.05 may not be rejected at α = 0.01 (fig. B1).

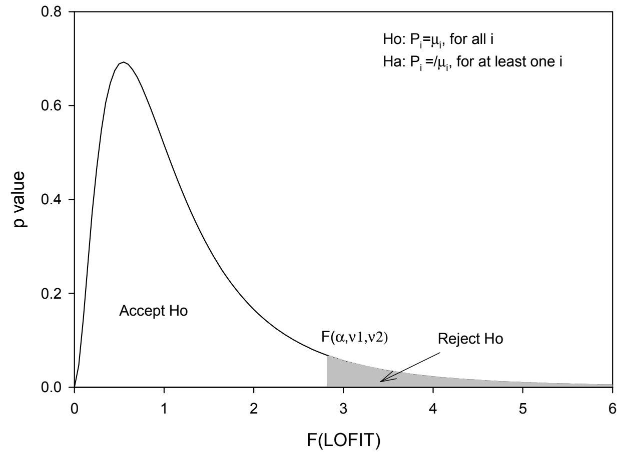

Figure B1. A diagram of the F(LOFIT) distribution.